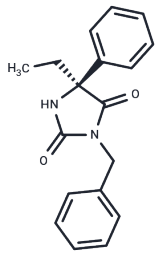
Data Sheet (Cat.No.T67926)

TargetMol

(S)-(+)-N-3-Benzylnirvanol

Chemical Properties



CAS No. : 790676-40-3

Formula: C18H18N2O2

Molecular Weight: 294.35

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	(S)-(+)-N-3-Benzylnirvanol is a cytochrome P450 CYP2C19 inhibitor with a ki value of 82.5μM for CYP2C9 and 0.25μM for CYP2C19, which can be used to study HIV infection.
Targets(IC50)	Others,HIV Protease,Cytochromes P450
In vitro	(S)-(+)-N-3-Benzylnirvanol is a cytochrome P450 CYP2C19 inhibitor with a ki value of 82.5μM for CYP2C9 and 0.25μM for CYP2C19.[1]

Solubility Information

Solubility	DMSO: 150 mg/mL (509.6 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (6.79 mM),Sonication is recommended. 10% DMSO+90% Saline: 10 mg/mL (33.97 mM),Suspension. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.3973 mL	16.9866 mL	33.9732 mL
5 mM	0.6795 mL	3.3973 mL	6.7946 mL
10 mM	0.3397 mL	1.6987 mL	3.3973 mL
50 mM	0.0679 mL	0.3397 mL	0.6795 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Suzuki H,et al. Active-site characteristics of CYP2C19 and CYP2C9 probed with hydantoin and barbiturate inhibitors. Arch Biochem Biophys. 2004 Sep 1;429(1):1-15.
Shirai F, et al. Design and Discovery of an Orally Efficacious Spiroindolinone-Based Tankyrase Inhibitor for the Treatment of Colon Cancer. J Med Chem. 2020;63(8):4183-4204.
Cuypers ML, et al. (-)-N-3-Benzylphenobarbital Is Superior to Omeprazole and (+)-N-3-Benzylnirvanol as a CYP2C19 Inhibitor in Suspended Human Hepatocytes. Drug Metab Dispos. 2020;48(11):1121-1128.

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